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Semiannual Status Report

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Statement of Work

The purpose of this program is to compile and initially evaluate diffusivity and viscosity data on gas, liquid, solid and turbulent flow systems. The program has been in operation for two years. Progress in the various areas of the program is discussed separately in the following sections.

I. Diffusion in Gases

The progress towards the critical evaluation of binary gas mixture diffusion coefficient measurements has continued as planned. A preliminary evaluation of almost all systems suitable for Standard Reference Data has been completed. Some additional diffusion coefficient data are being collected and all values retrieved will be included in the forthcoming final report.

Diffusion coefficient measurements for monatomic - monatomic systems (noble gas pairs) have been essentially all evaluated and correlated. The analyses of monatomic - polyatomic and polyatomic - polyatomic systems were recently completed, except for coefficients determined by the Stefan evaporation tube technique. The results were surveyed according to the experimental method, source and precision. Thus far, approximately seventy gas pairs have been evaluated. In addition to the Stefan measurements, it remains to review the weighting of each datum, then to correlate the results. Finally, estimates for quantum effects and composition dependences are to be made for all the gas pairs considered.

The noble gas diffusivity measurements will extend from at least the ice point to about 10,000°K. In the low temperature range, direct measurements of D are available; at the high temperatures, indirect values of D are obtained from molecular beam scattering experiments. The interpolation between these temperature ranges appears satisfactory for the majority of noble gas pairs. The application of kinetic theory, indirect measurements, and precis

graphs indicates that standard diffusion coefficients for the noble gas pairs may be specified from 273°K to 10,000°K, the uncertainty ranging from about 2% at the lower temperatures to about 10% of the higher temperatures.

The ultimate result of this critical evaluation of binary gaseous diffusion coefficient measurements will be a final report. As indicated, a considerable amount of data evaluation is presently outstanding. Another aspect not yet finally settled is the form in which the correlated diffusion coefficients should be presented. The use of simple equations is attractive, and power-law and Sutherland equations will be tried. Graphical smoothing and numerical tabulations are always possible as a last resort. We believe that our earlier estimate, that the final report can be written by the end of 1967, is still feasible.

II. Molecular Diffusion Coefficients - Binary Liquid Systems

The principle effort on the project during the current report period has been devoted to devising, and perfecting a data logging and retrieval system that will facilitate data storage and recall on a selective basis. Literature searching to bring the collected data up to date has been simultaneously been carried on, although at a somewhat reduced pace until the exact format of the data logging and retrieval system could be established.

The data retrieval program has been written for the IBM-7090-94 digital computer system of the University of Maryland using Fortran IV. If the search criteria demand, the program results in a tabular print-out as shown in the following illustration.

Each time a new page is required the program automatically starts a new page with the appropriate tabular headings. In order to facilitate data retrieval and search programs the solute and solvent names are codified according to the system used by the "Thermophysical Properties Review Center" system (Purdue University -

Figure No

DIFFUSION & VISCOSITY COEFFICIENTS IN BINARY LIQUID SYSTEMS

Temp. °C	Solute Concentration	Diffusion Coefficient $x10^5 cm^2/sec$	Diffusion Type Coeff. Method	Precision	Reference for Diff.Coeff.	Viscosity Coefficient	Reference for Viscosity

Solvent Name and Code Number

Solute Name and Code Number

_____ Lines of data _____

_____ Lines of data _____

(etc)

Solvent Name and Code Number

Solute Name and Code Number

_____ Lines of data _____

_____ Lines of data _____

_____ Lines of data _____

(etc)

Dr. Toloukian). An information print-out will precede each table. The text in this print-out will describe the table and give directions for its efficient use; i.e. explain the coding system and the use of footnotes for those systems departing from the simple format of the tabulation. The program will handle systems of the type wherein a solute diffuses through a binary solvent --- thus representing a ternary system.

Data are read by the program which defines the search criteria. The program first checks the solute and solvent codes --- if these data conform to the search criteria the program then checks each line of data information. If a line of data meets all the search criteria it results in a print-out in the tabular form. In this manner, the data cards (or tape) may be searched for any particular component (solute or solvent) or combination of components, for a series of experimental type measurements or methods, for particular data characteristics, or for individual references. In essence any of the tabular information may be used as search criteria.

At the present time the accumulated data is being codified and placed on cards in accord with the program format. The 1966 data collected is being used to test the program and smooth out the operational bugs that appear. The final program should be completely debugged within the next month, enabling us to begin the massive task of coding all the data in the desired form, and preparing some sample print-outs.

Along with the above programming activities, data collection is being continued from the published literature and we are also contacting private industrial companies to determine if they have research data they will permit to be included in the program.

III. Diffusion in Inorganic Solids

The re-evaluation of the diffusion coefficient for **AgCl** is now complete and a short note is being prepared for publication to correct the erroreous equation presented in the literature. Mean-

while our compilation of alkali halide data is continuing. The literature in this field is very large and active and a considerable amount of effort is required to plot and correlate the various data. We are hopeful that we can complete this correlation soon and then undertake a critical review for the selection of best available equations representing the self-diffusion rates in alkali halides.

IV. Diffusion in Polymer-Diluent Systems

The program of compiling and evaluating diffusion coefficients in polymer diluent systems has reached the point where we have abstracted the bulk of the data in the available literature and are preparing to analyze the data. Data are available on more than 70 polymers and more than 70 diluents. The task of evaluating and correlating the data is difficult because many sytems have not been adequately described. Several reports have been published in which none of the physical or chemical properties of the polymer are listed. Correlation and comparison of data found in reports of this type can not be justified.

Those systems which have been adequately described are to be statistically correlated using the OMNITAB computer program. The program will be used to reduce the data to tabular form and to place confidence limits on the temperature dependence of the diffusion coefficient. When sufficient data are available for a particular penetrant - polymer pair an attempt will be made to correlate the effect of polymer density and penetrant diffusivity.

V. Turbulent Transport Coefficients

The initial phase of the project is essentially complete. We have copies of nearly all publications during the past ten years containing turbulent transport data. Work has begun on the second phase of abstracting and evaluating the data. This process of compilation and evaluation will represent the major effort during

the next period. We feel that we can meet our original estimate of having a final report ready during 1968.

VI. Personnel

The investigation of diffusion in gases is directed by Dr. E. A. Mason. He is assisted by one graduate student, Mr. T. R. Marrero.

The liquid diffusion survey is directed by Dr. R. B. Beckmann, with the assistance of two graduate students, Mr. D. J. Harris and Mr. P. N. Vashist, a part-time research associate, Mrs. M. C. Bailey, and a part-time student, Miss Caroline Ugiansky.

The investigation of diffusion in inorganic solids is directed by Dr. L. P. Skolnick, he is assisted by one graduate student, Mr. L. Slawecki.

The polymer diffusion survey is directed by Dr. T. G. Smith, with the assistance of a graduate student, Mr. Ronald Heck.

Dr. J. M. Marchello is directing the turbulent transport survey and is assisted by one graduate student, Mr. E. F. Logan.